PROGRESS REPORT

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2. HITRAN Database Developments for ARM

3. The goal of this research effort is to provide the ARM community with an archival database of spectroscopic parameters that will serve as input to atmospheric radiation modeling codes. The database is the HITRAN compilation which includes molecular spectroscopic parameters for simulating absorption and radiance by gases in the atmosphere, infrared cross-sections for gases with dense spectral features, aerosol indices of refraction, and associated software to enable ARM users to easily extract information relevant to their problems. The data compiled for HITRAN are obtained from both quantum mechanical calculations and also directly from laboratory measurements.

   A major concern for the ARM program is the reliability of water-vapor spectroscopic parameters, especially the intensity of lines in the near-IR and visible regions. The HITRAN program will evaluate and validate new laboratory observations of water-vapor spectra. New theoretical techniques for the prediction of weak water-vapor absorptions applicable to long-path simulations needed by the ARM program will also be investigated and implemented. Upon validation, new parameters will be made available in the HITRAN format and placed in the HITRAN web-site prior to release on the archival, CD-ROM media.

4. ♦ NASA Ames Research Center water-vapor data fixed and put on web-site.

   ♦ Special Session on water-vapor spectroscopic parameters held at HITRAN Database Conference at Harvard-Smithsonian.

5. Many water-vapor line intensities in the region from 8000 to 23,000 $cm^{-1}$ (1.25 to 0.435 micrometers) have been modified. This work was accomplished through the study of L.P. Giver, C. Chackerian Jr., and P. Varanasi, *J. Quant. Spectrosc. and Rad. Transfer*. **66,** 101-105 (2000). The group at NASA Ames have been making new measurements of water vapor in this region and noticed discrepancies between the intensities in the current edition of HITRAN (L.S. Rothman et al, *J. Quant. Spectrosc. and Rad. Transfer*. **60,** 665-710 (1998)) and their observations. An analysis going back to the original observations used for HITRAN revealed some corrections for unit conversion had not been uniformly applied. The original data came from five separate publications, although all observations were taken using the facility at Kitt Peak National Solar Observatory. In creating a new line list for this region, the corrections to the intensity were applied and some lines which were previously

unidentified have also been assigned using the ab initio calculations of Schwenke (D. Schwenke, *J. Mol. Spectrosc.* **190,** 397-402 (1998)). The file sent to us from NASA Ames was put into the HITRAN format, and some minor errors, such as duplicated lines, were removed. References were placed on the lines, and the file was set up as a total replacement for water vapor in HITRAN above 8000 $cm^{-1}$. The file has been placed on the HITRAN web-site for access by users. The halfwidths remain the same as in the standard edition of HITRAN.

The Sixth HITRAN Database Conference was held at the Harvard-Smithsonian Center for Astrophysics 19-21 June 2000. Over 70 colleagues attended the conference. Almost one-third of the attendees were from abroad. The conference consisted of oral presentations and poster sessions. The first day was devoted primarily to issues involving the database and remote sensing. The second day was devoted to new spectroscopic parameters. On the last day of the conference, a special session was held dedicated to water-vapor spectroscopy. There were eight invited oral presentations in this session. The session covered theoretical treatments, new observations in the thermal infrared, new assignments for lines in the visible region, weak line observations and theoretical treatments in the near-IR and visible taken in the UK, the laboratory spectra performed by JPL, and halfwidth measurements made at Stony Brook. In addition, there was a relevant talk on the whole question of the process of going from the raw data to the derived parameters.

6. It is to be understood that the update for water vapor placed on the web-site is an interim enhancement to the HITRAN database. It only makes corrections to old data that were taken in the early '80s. We are currently in a program with the Jet Propulsion Laboratory to provide new data for water vapor in several spectral regions. Preliminary data in the near-IR and short wavelength region have recently been produced by Dr. Linda Brown of JPL. We are currently processing these data for the HITRAN database and are validating them. There are additional data from Dr. Robert Toth of JPL in the 500 to 2800 $cm^{-1}$ region. These data include the three isotopomers with oxygen 16, 17, and 18 as well as the deuterated species HDO.

   We have updated the strength calculations for the rotational bands of two minor isotopomers of $H_2O$ (the $H_2{}^{17}O$ and $H_2{}^{18}O$ molecules) using the model of John Pearson at JPL. These calculations cover the entire far infrared region (0-1000 $cm^{-1}$). These calculations have been used for atmospheric retrievals of the minor isotopomers. The atmospheric concentration retrievals from individual transitions are much more consistent than with the older calculations in the current HITRAN release. These retrievals also give more consistent concentration profiles when compared to the main isotopomer of $H_2O$ in the context of atmospheric circulation models. More improvement on these calculations are expected in the future.

7. None (current grant commenced November 1999).

8. "Atmospheric Molecules," L.S. Rothman and M. Zivkovic-Rothman, Proceedings of ICAMDATA (International Conference on Atomic and Molecular Data), Oxford, UK, American Institute of Physics (2000).

   Proceedings of the Sixth Biennial HITRAN Database Conference, Harvard-Smithsonian Center for Astrophysics, Cambridge MA, USA (2000).

9. "Total Internal Partition Sums for Molecules in the Terrestrial Atmosphere," R.R. Gamache, S. Kennedy, R.L. Hawkins, and L.S. Rothman, *Journal of Molecular Structure* **517/518,** 413-431 (2000).

"HITRAN Partition Functions and Weighted Transition-Moments Squared," A. Goldman, R.R. Gamache, A. Perrin, J.-M. Flaud, C.P. Rinsland, and L.S. Rothman, *J. Quant. Spectrosc. and Rad. Transfer*. **66,** 455-486 (2000).